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Structural and elastic properties of zinc-blende and wurtzite $InN_{1-x}Bi_x$ alloys

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Abstract

Structural and elastic properties of $InN_{1-x}Bi_x$ alloys in both zinc-blende and wurtzite phases are studied by using first-principle calculations. Two different Bi-atom arrangements of uniform and clustered configurations have been considered for x=0.25, 0.5, and 0.75. It is found that clustered configuration has a significant effect on lattice parameters of wurtzite $InN_{1-x}Bi_x$ alloys. A slightly sublinear dependence on the alloy content, x, can be accepted for C_{11}, C_{12}, C_{13}, and C_{33} in zinc-blende $InN_{1-x}Bi_x$, and for C_{12}, C_{13}, and C_{44} in wurtzite $InN_{1-x}Bi_x$, whereas clearly linear deviations are obtained for C_{44} and C_{66} in zinc-blende alloys and for C_{11} and C_{33} in wurtzite alloys. The effect of Bi atoms clustering leads to a decrease in all elastic constants and bulk modulus in zinc-blende $InN_{1-x}Bi_x$, and makes big deviations from Vegard's-like law and has little influence on bulk modulus in wurtzite $InN_{1-x}Bi_x$ alloys.

Keywords: zinc-blende; wurtzite; clustered arrangement; $InN_{1-x}Bi_x$; elastic constant**.**

1. Introduction

The group-III nitrides have been the focus of intensive concern because of their